$C_{10}H_{21}$—$I^-$—$N^+$—$(CH_2)_2$—$N^+$—$I^-$—$C_{10}H_{21}$
DQ 9I

$C_{10}H_{21}$—$Cl^-$—$N^+$—$(CH_2)_6$—$N^+$—$Cl^-$—$C_{10}H_{21}$
DQ 10Cl

$C_{10}H_{21}$—$I^-$—$N^+$—$(CH_2)_6$—$N^+$—$I^-$—$C_{10}H_{21}$
DQ 10I

$C_{18}H_{37}$—$Cl^-$—$N^+$—$(CH_2)_2$—$N^+$—$Cl^-$—$C_{18}H_{37}$
DQ 11Cl

$C_{18}H_{37}$—$I^-$—$N^+$—$(CH_2)_2$—$N^+$—$I^-$—$C_{18}H_{37}$
DQ 11I

$C_{18}H_{37}$—$Cl^-$—$N^+$—$(CH_2)_6$—$N^+$—$Cl^-$—$C_{18}H_{37}$
DQ 12Cl

$C_{18}H_{37}$—$I^-$—$N^+$—$(CH_2)_6$—$N^+$—$I^-$—$C_{18}H_{37}$
DQ 12I

$C_{18}H_{37}$ — $Cl^-$ N+ ... +N $Cl^-$ — $C_{18}H_{37}$
DQ 13Cl

$C_{18}H_{37}$ $I^-$ N+ ... +N $I^-$ — $C_{18}H_{37}$
DQ 13I

$C_{10}H_{21}$ — $Cl^-$ N+ ... +N $Cl^-$ — $C_{10}H_{21}$
DQ 14Cl

$C_{10}H_{21}$ $I^-$ N+ ... +N $I^-$ — $C_{10}H_{21}$
DQ 14I

$C_{18}H_{37}$—$Cl^-$—$N^+$—$(CH_2)_4$—$N^+$—$Cl^-$—$C_{18}H_{37}$
DQ 15Cl

$C_{18}H_{37}$—$I^-$—$N^+$—$(CH_2)_4$—$N^+$—$I^-$—$C_{18}H_{37}$
DQ 15I

$C_{18}H_{37}$—$Cl^-$—$N^+$—$(CH_2)_3$—$N^+$—$Cl^-$—$C_{18}H_{37}$
DQ 17Cl

$C_{10}H_{21}$—$I^-$—$N^+$—$(CH_2)_4$—$N^+$—$I^-$—$C_{10}H_{21}$
DQ 16I

$C_{10}H_{21}$—$Cl^-$—$N^+$—$(CH_2)_3$—$N^+$—$Cl^-$—$C_{10}H_{21}$
DQ 18Cl

$C_{18}H_{37}$—$I^-$—$N^+$—$(CH_2)_3$—$N^+$—$I^-$—$C_{18}H_{37}$
DQ 17I

$C_{10}H_{21}$—$I^-$—$N^+$—$(CH_2)_3$—$N^+$—$I^-$—$C_{10}H_{21}$
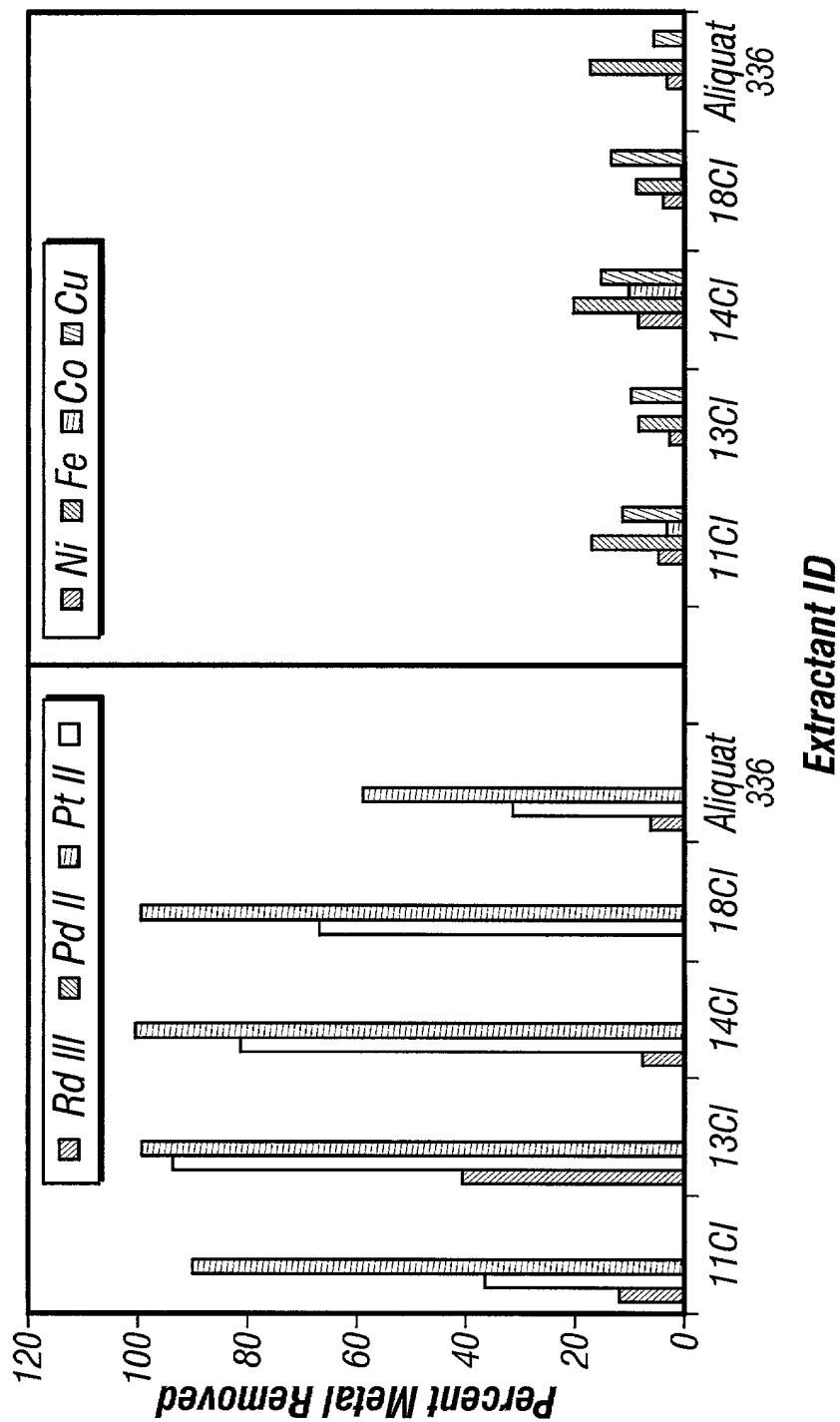DQ 18I

**FIG. 1**

*FIG. 2*

| Compound | D-Value Pd II | Conformation Minimum Energy (kcal/mole) | Connectivity Index (order 2, standard) D | Dipole Moment (debye) E | Electron Affinity (eV) F |
|---|---|---|---|---|---|
| DQ 18 | 2.86 | 39.331 | 11.632 | 12.744 | 7.127 |
| DQ 16 | | 39.449 | 11.985 | 2.933 | 6.601 |
| DQ 10 | 1.75 | 40.322 | 12.692 | 0.01 | 5.948 |
| DQ 14 | 2.6 | 39.924 | 11.071 | 25.323 | 8.122 |
| DQ 17 | 3.3 | 50.797 | 17.289 | 25.52 | 7.139 |
| DQ 15 | 0.42 | 49.902 | 17.642 | 0.025 | 6.597 |
| DQ 12 | 1.59 | 50.899 | 18.349 | 0.124 | 5.946 |
| DQ 13 | 3.22 | 50.293 | 16.728 | 52.726 | 8.119 |
| DQ11 | 0.89 | 49.694 | 16.935 | 0.148 | 7.867 |

FIG. 3A

| Compound | Dielectric Energy (kcal)/mole) G | Steric Energy (kcal/mole) H | Total Energy (Hartree) I | Heat of Formation (kcal/mole) | HOMO Energy (ev) |
|---|---|---|---|---|---|
| DQ 18 | 7.7 | 39.331 | 214.593 | 258.295 | 13.703 |
| DQ 16 | 7.211 | 39.597 | 221.775 | 242.427 | 13.635 |
| DQ 10 | 6.602 | 40.322 | 236.121 | 218.102 | 13.52 |
| DQ 14 | 8.438 | 39.924 | 205.938 | 291.32 | 13.855 |
| DQ 17 | 7.759 | 50.797 | 329.153 | 171.131 | 12.628 |
| DQ 15 | 7.301 | 49.902 | 336.331 | 155.69 | 12.601 |
| DQ 12 | 6.62 | 50.899 | 350.679 | 131.143 | 12.552 |
| DQ 13 | 8.487 | 50.293 | 320.496 | 204.337 | 12.687 |
| DQ11 | 8.312 | 49.694 | 321.968 | 190.296 | 12.661 |

*FIG. 3B*

| Compound | Ionization Potential (eV) L | Log P M | LUMO (eV) Energy N | Shape Index (basic kappa, order 3) O | Valence Connectivity Index (order 2, standard) Q | Solvent Accessible Surface Area ($Å^2$) P |
|---|---|---|---|---|---|---|
| DQ18 | 13.703 | 6.409 | -7.127 | 21.031 | 521.24 | 11.069 |
| DQ16 | 13.635 | 6.86 | -6.601 | 22.027 | 539.815 | 11.423 |
| DQ10 | 13.52 | 7.653 | -5.948 | 23.967 | 576.054 | 12.13 |
| DQ14 | 13.855 | 6.179 | -8.122 | 13.04 | 485.397 | 10.53 |
| DQ17 | 12.628 | 12.75 | -7.139 | 36.681 | 813.7 | 16.726 |
| DQ15 | 12.601 | 13.201 | -6.598 | 37.686 | 831.853 | 17.08 |
| DQ12 | 12.552 | 13.993 | 5.946 | 39.658 | 883.721 | 17.787 |
| DQ13 | 12.687 | 12.52 | -8.119 | 26.747 | 778.615 | 16.187 |
| DQ11 | 12.661 | 12.697 | -7.867 | 35.716 | 793.278 | 16.372 |

*FIG. 3C*
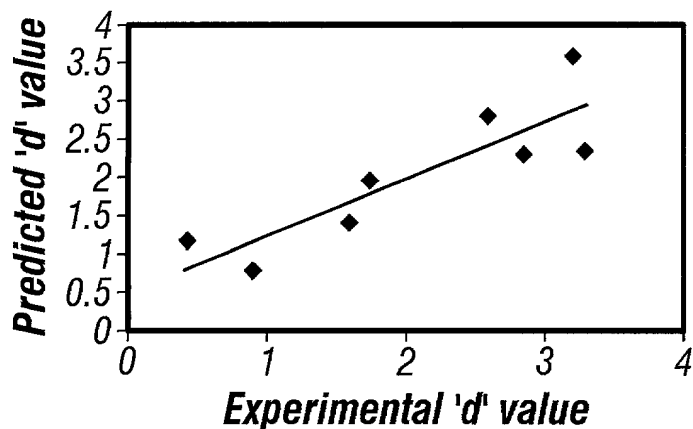
Predictive Eq. for Pd II

$B=0.0554277*E+0.610452*L-16.7616/N-9.0729$

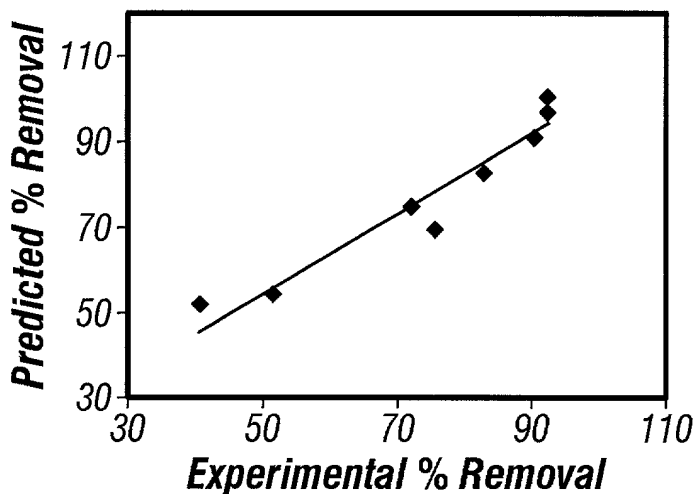**FIG. 4A**
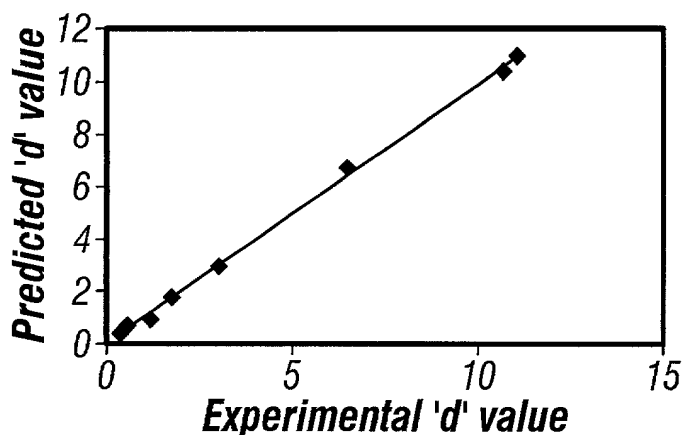


Predictive Eq. for Pd IV
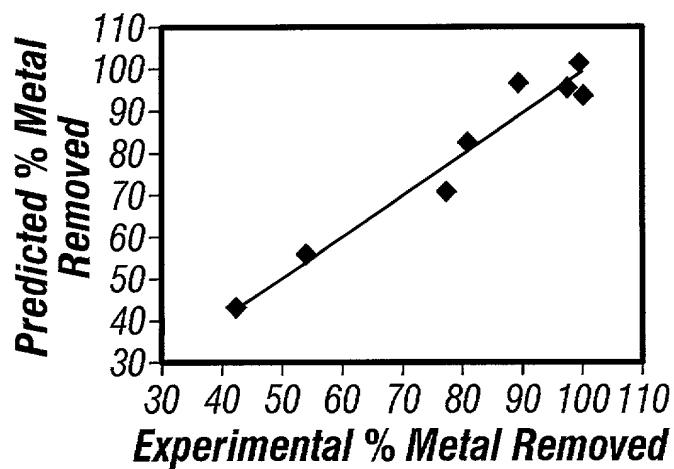
$B=71.6336*D+0.463796*E+23.6272*F+19.8848*G-9.37422*H+2.71931*I+108.256$

**FIG. 4B**



Predictive Eq. for Pt II

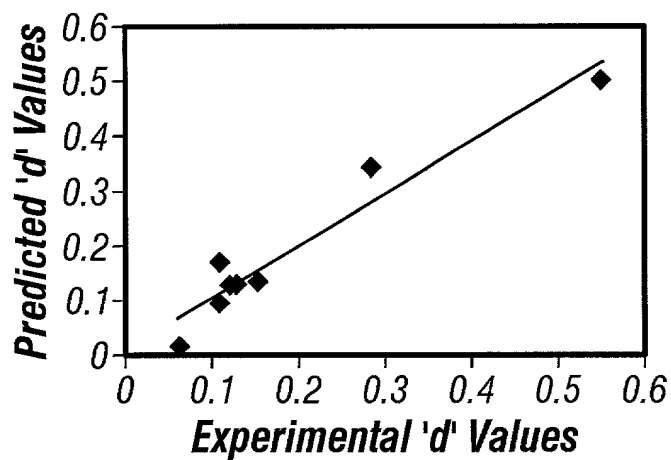$B=-276.194*L-69.6714*M-4.68162*N-7.67628*O+3.7778*P-154.864*Q+4211.14$

**FIG. 4C**

Predicted % Metal Removed

110
100
90
80
70
60
50
40
30

30 40 50 60 70 80 90 100 110

**Experimental % Metal Removed**

Predictive Eq. for Pt IV

B=283.378*D+1.4239
9*E+173.825*F+212.2
66*G+2.69479*H+14
4354*I+167.3

*FIG. 4D*

Predicted 'd' Values

0.6
0.5
0.4
0.3
0.2
0.1
0

0   0.1   0.2   0.3   0.4   0.5   0.6

**Experimental 'd' Values**

Predictive Eq. for Rh III

B=0.00584793*E-
0.90334*N-42.1486/N-
12.3346

*FIG. 4E*

Dissolve metals from catalytic converter in 3M HCl

| (PPM) | Pd | Pt | Al | Cu | Fe | Cr | Ni | Pb |
|---|---|---|---|---|---|---|---|---|
| | 67.6 | 594 | 3237 | 27 | 196 | 5 | 5 | 142 |

Extract Pd selectively with KI treatment

| (PPM) | Pd | Pt | Al | Cu | Fe | Cr | Ni | Pb |
|---|---|---|---|---|---|---|---|---|
| | 0.77 | 594 | 3237 | 27 | 196 | 5 | 5 | 142 |

Extract Pt selectively with 5% diquat solution

| (PPM) | Pd | Pt | Al | Cu | Fe | Cr | Ni | Pb |
|---|---|---|---|---|---|---|---|---|
| | 0.77 | 297 | 3237 | 27 | 186 | 5 | 5 | 124 |

Extract metals with (Q)ALIQUAT336 & (M)ALAMINE336

| (PPM) | Pd | Pt | Al | Cu | Fe | Cr | Ni | Pb |
|---|---|---|---|---|---|---|---|---|
| Q | 38.4 | 594 | 3247 | 27 | 182 | 5 | 5 | 142 |
| M | 47 | 594 | 3247 | 27 | 182 | 5 | 5 | 142 |

FIG. 5